

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 753 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.97e-01

Confidence level: 7.05e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Fenarimol</div> <div>Measured: 603</div> <div>Predicted: 753</div>	<div>Image not found</div> <div>Chlorobenzilate</div> <div>Measured: 2000</div> <div>Predicted: 824</div>	<div>Image not found</div> <div>Warfarin</div> <div>Measured: 912</div> <div>Predicted: 1080</div>
<div>Image not found</div> <div>Ethofumesate</div> <div>Measured: 339</div> <div>Predicted: 178</div>	<div>Image not found</div> <div>Naptalam-sodium</div> <div>Measured: 2190</div> <div>Predicted: 1690</div>	